CONTENTS

Symmetry analysis of the electronic structure of polyhedron clusters M_{12} (I_h), M_{12} (O_h) and M_{60} (I_h)
B.-C. Wang (Tamsui, Taiwan) and Y.-N. Chiu (Washington, DC, USA) 1
Additive properties of electron density in diatomic homonuclear molecules: application to the hydrogen molecule
K. Tkacz and W.S. Ptak (Kraków, Poland) 21
Construction of orthogonalized maximum overlap symmetry orbitals
C.-G. Zhan (Wuhan, People's Republic of China) 33
Construction of the symmetry orbitals in large molecular systems
C.-G. Zhan (Wuhan, People's Republic of China) 39
Maximum overlap population principle and direct calculation of bond order, valence and atomic charge
C.-G. Zhan (Wuhan, People's Republic of China) 47
The maximum overlap symmetry orbital method and the group overlap method
C.-G. Zhan (Wuhan, People's Republic of China) 57
Structural stability and energetics of sulphur microclusters: an MNDO calculation
H. Yilmaz and S. Erkoç (Ankara, Turkey) 63
The interaction of a laser pulse with a periodic quasi-one-dimensional polymer
J.J. Ladik and L.R. Dalton (Los Angeles, CA, USA) 77
Ab initio calculations of the equilibrium geometries and vibrational frequencies of carbonyl cyanide, thiocarbonyl cyanide and thiopropynal
J. Tyrrell (Carbondale, IL, USA) 87
NDDO and ab initio molecular orbital studies of vapor phase complexes between HF and AlF_3 molecules
G. Scholz, D. Menz and L. Kolditz (Berlin, Germany) and C. Nieke (Leipzig, Germany) 95
MINDO/3 and MNDO studies of some thio analogues of nucleic acid bases
K. Singh and D.K. Rai (Varanasi, India) and J.S. Yadav (Newark, NJ, USA) 103
Theoretical calculations of β-lactam antibiotics. Part 1. AM1, MNDO and MINDO/3 calculations of some penicillins
J. Frau, M. Coll, J. Donoso and F. Muñoz (Palma de Mallorca, Spain) and F. García Blanco (Madrid, Spain) 109
Transition states for molecular hydrogen elimination from substituted silanes
G.J. Mains (Stillwater, OK, USA), M. Trachtman and C.W. Bock (Philadelphia, PA, USA) ... 125
Gradient-optimised geometries of a trans and a gauche conformation of haloperidol at the 4-21G level: comparison of the piperidino unit with gas phase piperidine
A. Peeters, C. Van Alsenoy, A.T.H. Lenstra and H.J. Geise (Wilrijk, Belgium) 137
Nature of potential energy surface modification in reactions of formation and destruction of ion triplets $HCOO^- \cdot 2Me^+$
A.M. Kariev and A.A. Ovchinnikov (Moscow, USSR) 151
Ab initio study of the molecular structure of linear furocoumarins and pyrrolocoumarins
C.M. Estévez, A.M. Graña, M.A. Ríos and J. Rodríguez (Santiago de Compostela, Spain)... 163
Electroreduction of β-chloropropiophenone: a study of stability of cis and trans isomers of 1,5-diphenyl-2,6-dioxa[3,3,0]bicyclooctane and on the logical reaction pathway
V.G. García, F. Cases, V. Montiel, E. San Fabián and A. Aldaz (Alicante, Spain) 169
A model for the hydrogen-bonding interactions between adenosine receptor ligands and histidyl residues in the adenosine A_1 receptor binding site, based on AM1 calculations
E.M. Van Der Wenden, P.J.M. Van Galen, A.P. IJzerman and W. Soudijn (Leiden, The Netherlands) 175
How reliable are ab initio calculations? The structure and conformation of chlorocarbonyl isocyanate (ClC(O)NCO) revisited
M.T. Nguyen, M.R. Hajnal and L.G. Vanquickenborne (Leuven, Belgium) 185
Geometry changes with ionization in diphenyl sulfide
G.F. Musso, P. Piaggio and G. Dellepiane (Genova, Italy) and A. Borghesi (Pavia, Italy) 195

Semi-empirical molecular orbital calculations on tyrosine kinase inhibitors and structurally related compounds
P.C. Yates (Birmingham, UK) 201
On relative stability interchange between H–O and H–N bonded heterodimers of nitrous oxide and water
Z. Slanina (Mainz, Germany) 215
On the classification and enumeration of planar polyhex hydrocarbons
S. Nikolić and N. Trinajstić (Zagreb, Yugoslavia), J.V. Knop, W.R. Müller and K. Szymanski (Düsseldorf, Germany) 219
Calculations of magnetic susceptibility of some molecules by the variational method using ab initio wave functions
R.M. Aminova and G.K. Zakirova (Kazan, USSR) 227
Interchain interaction of ^{13}C NMR chemical shift and electron structure of polypeptide chains in the solid state as studied by tight-binding MO theory: poly(L-alanine) with the right-handed and left-handed α-helix forms
H. Kurosu and I. Ando (Tokyo, Japan) 231
The low-lying electronic states of cerium monoxide CeO: ab initio calculations using energy-adjusted pseudopotentials and spin–orbit operators
M. Dolg, H. Stoll and H. Preuss (Stuttgart, Germany) 243
Semi-empirical molecular orbital calculations on pyrimidine-2-thiol and pyrimidine-2-thione: prototropic tautomerism
J.G. Contreras and J.B. Alderete (Concepción, Chile) 257
Ab initio calculations of the properties of the CNH···NCH and C_3NH···NCH linear complexes
J. Bosco, P. da Silva and M.N. Ramos (Recife, Brazil) 267
Electron correlation effects on the energy band structure of polyglycine
P. Otto and A. Sutjianto (Erlangen, Germany) 277
Ab initio study of 1,4-dithiin and its cation radical and dication
T. Nakano, K. Morihashi and O. Kichuchi (Tsukuba, Japan) 283
Internal coordinate approach for the vibrational predissociation of $(NO)_2$
A. Tachibana, M. Yamato, T. Suzuki and T. Yamabe (Kyoto, Japan) 291
Stability of the molecular anions ClO_4^-, HCO^- and O_3^- from the self-interaction corrected multiple-scattering Xα method
Y. Guo and M.A. Whitehead (Montreal, Que., Canada) 307
The *k*-resonant benzenoid systems
M. Zheng (New Brunswick, NJ, USA) 321
Valence bond order and superconductivity
E.W. Kvam (New York, NY, USA) 335
MNDO studies on the structure of Antineoplaston A10, glutarimide and piperidine
D. Michalska (Wrocław, Poland) 357
Set spectra of chemical spaces
L. Schulz (Poznań, Poland) 367

Short Communication
Comment on the paper: Kekulé count and algebraic structure count for unbranched alternant cata-fusenes, J. Mol. Struct. (Theochem), 179 (1988) 99
P.E. John (Ilmenau, Germany) 379

Announcement 383

Erratum 385

Author Index 387

Subject Index 389